Deformation of Low Symmetry and Multiphase Materials

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Materials composed of low symmetry crystals or of multiple solid phases exhibit heterogeneous deformation at the microstructural scale, presenting significant challenges to efforts to construct macroscale constitutive models. This deformation heterogeneity at the microstructural scale also produces stress concentration, which can lead to fracture or influence the onset and progress of phase transformations. We are developing an approach that explicitly incorporates effects of microstructure and deformation heterogeneity in a framework suited to analysis of engineering scale components.

Applications involving fully developed plastic flow are targeted. We explicitly represent the microstructure, directly treating deformation heterogeneities, and we build on emerging technologies for effectively combining microscale plasticity simulations with macroscale models. New capabilities will capture the impact of microstructure, and thus material processing, on performance of engineering scale components. For example, phenomena such as shear localization arise naturally from application of the method at the appropriate scale.

Project Goals

The overarching goal of this project is to produce effective macroscale models through novel homogenization methods for materials where conventional methods fail. The immediate application space includes a broad class of engineering simulations, ranging from forming operations to dynamic loading scenarios. Figure 1 shows an example application, with computation performed using similar techniques appropriate to single-phase cubic symmetry polycrystalline materials. Software is developed in a component-oriented fashion, making use of tools that enhance parallel load-balancing through task parallelism, as shown in Fig. 2. Initial development is focused on the Ti-6%Al-4%V (Ti-6Al-4V) alloy, given its widespread use and the availability of relevant experimental data.

Relevance to LLNL Mission

In multiphase materials of interest to LLNL, such as Ti-6Al-4V, microstructure influences yield and flow stresses, ductility, high- and low-cycle fatigue, creep, fracture toughness, and large crack growth properties. Microstructure has also been shown to influence response under dynamic loading conditions. The presence of low symmetry phases can contribute to severe anisotropy and a tendency for strain localization. Explicit inclusion of the microstructure allows for the effective treatment of deformation heterogeneities at the microstructural scale. In addition to multiphase titanium alloys, the approach is applicable to low symmetry crystalline metals such as uranium (orthorhombic), beryllium (hexagonal), and α-plutonium (monoclinic).

FY2007 Accomplishments and Results

Our first completed milestone is associated with the assessment of important features for microstructures of interest in Ti-6Al-4V. We are able to use experimental data to inform numerical multiphase microstructure realizations (Fig. 3). New techniques have been developed to capture the morphology of the experimentally observed microstructures.

Another milestone is associated with new capabilities for fine-scale calculations in the ALE3D finite element program. We have determined a fine-scale implementation strategy and have tested ALE3D in the role of the fine-scale model. New capabilities have been developed for obtaining steady plastic flow solutions in ALE3D, with a specialized elasto-viscoplastic fine-scale material model. Figure 4 depicts results from an example calculation performed using ALE3D.

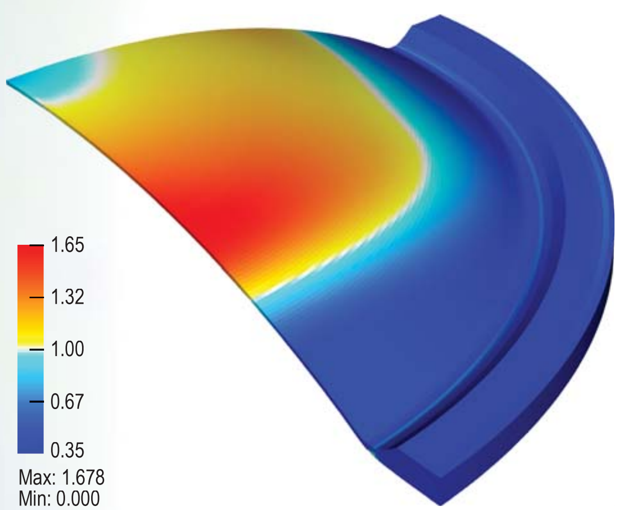

Figure 1. A biaxial bulge test workpiece, deformed by application of pressure to the lower surface. The false color depicts the relative effective plastic strain rate. Due to its lattice orientation distribution function, the sheet material has orthotropic symmetry and exhibits macroscopic strain localization, as indicated by the red region along the nearer symmetry plane.

Implementation is under way for new physics and software requirements for the appropriate coarse/fine coupling strategy. This includes homogenization to obtain anisotropic coarse-scale elastic response from fine-scale data, new coupling software for fine-scale models that do not provide derivative information, and velocity-gradient-driven parameterized plastic flow.

Related References

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3. Barton N. R., and H.-R. Wenk, "Dauphiné Twinning in Polycrystalline Quartz," *Modeling Simul. Mater. Sci. Eng.*, **15**, pp. 369-394, 2007.

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FY2008 Proposed Work

In the coming fiscal year, software components that have been developed for various aspects of the multiscale problem will be combined into a working whole. After testing, algorithm refinement, performance tuning, and model calibration, the overall capability will be validated by comparison with available experimental data at the appropriate length scale. We also plan to demonstrate extension of the method to another low symmetry or multiphase material such as beryllium or uranium.

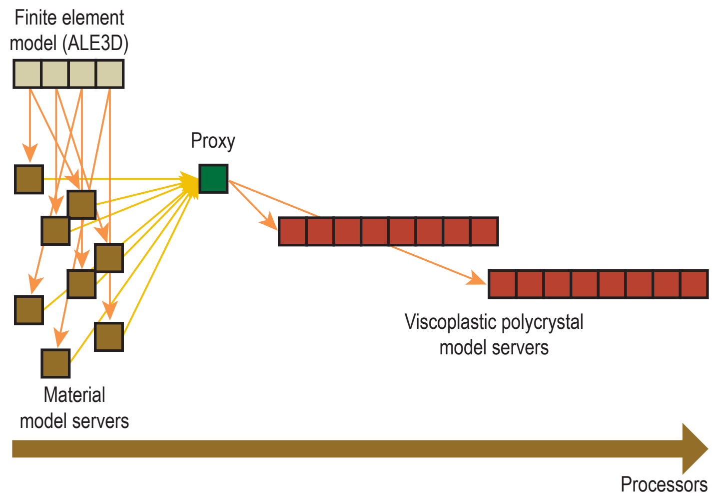

Figure 2. Schematic of Multiple-Program, Multiple-Data (MPMD) parallelism showing the Remote Method Invocation (RMI) pattern during the material model evaluation. Each box indicates a separate instance of a given executable program, with box subdivisions indicating parallelism within an executable.

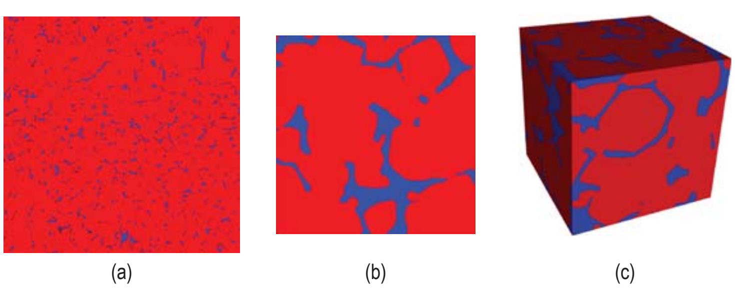

Figure 3. (a) Measured, (b) and (c) numerically generated (at different magnifications) microstructures for Ti-6Al-4V. Red indicates α phase; blue indicates β phase. Microstructures are obtained experimentally using electron backscatter diffraction. Numerical microstructures are generated by sampling the appropriate distribution functions and using particle-packing techniques. Numerical microstructures reproduce experimentally observed morphologies, with tunable parameters to control features such as phase volume fraction.

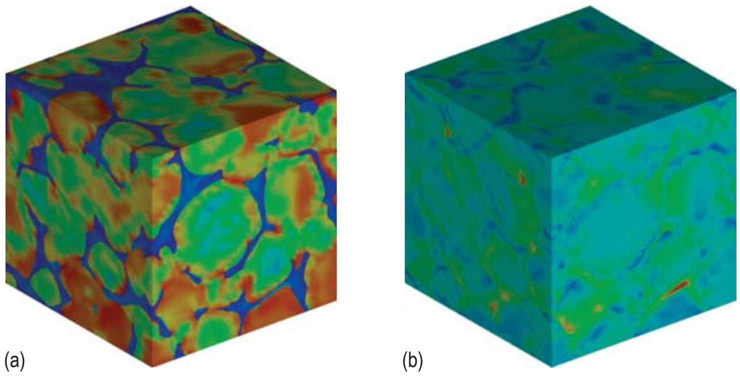

Figure 4. Heterogeneity of (a) stress magnitude and (b) plastic strain rate in a two-phase Ti-6Al-4V microstructure simulated in ALE3D, with relative plastic strain rates reaching ten times the nominal applied value. The highest relative plastic strain rates are observed in the β phase, which has a more isotropic flow behavior, while the highest stress magnitudes are observed in the more anisotropic α phase.